Abstract Submitted for the MAR05 Meeting of The American Physical Society

Solvent-induced collapse of a helical semiflexible polymer VIKAS

VARSHNEY, GUSTAVO A. CARRI, The University of Akron — It has been stated that "the class of materials richest in the occurrence of phase transitions are polymers" (E. A. Di Marzio, *Prog. Polym. Sci.* 24, 329 (1999)). This wealth of phase transitions is unique to polymers and is a consequence of the myriad of possible ways of coupling the basic ten classes of polymeric phase transitions into pairs, triplets and so forth. Two of these transitions are the helix-coil and coil-globule transitions. In this talk we explore the coupling of these two transitions, its molecular origins and physical consequences. For this purpose, we extend a recently developed model of helical polymers to describe the effect of solvent quality and solve it using Monte Carlo simulations based on the Wang and Landau algorithm. We find a very rich phase diagram consisting of 6 phases characterized by very specific conformations of the chain, i.e., a perfect helix, a random coil, a globule or other globular states with residual helical strands. We study the phase boundaries and provide further insight into the physics of the problem with a detailed analysis of the conformational and thermodynamic properties of the polymer chain.

Vikas Varshney The University of Akron

Date submitted: 28 Nov 2004 Electronic form version 1.4